

1 **Optimization of a radiative transfer forward operator for**
2 **simulating SMOS brightness temperatures over the Upper**
3 **Mississippi Basin, USA**

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ABSTRACT

The Soil Moisture and Ocean Salinity (SMOS) satellite mission is routinely providing global multi-angular observations of brightness temperature (TB) at both horizontal and vertical polarization with a 3-day repeat period. The assimilation of such data into a land surface model (LSM) may improve the skill of operational flood forecasts through an improved estimation of soil moisture (SM). To accommodate for the direct assimilation of the SMOS TB data, the LSM needs to be coupled with a radiative transfer model (RTM), serving as a forward operator for the simulation of multi-angular and multi-polarization top of atmosphere TBs. This study investigates the use of the Variable Infiltration Capacity (VIC) LSM coupled with the Community Microwave Emission Modelling platform (CMEM) for simulating SMOS TB observations over the Upper Mississippi basin, USA. For a period of 2 years (2010-2011), a comparison between SMOS TBs and simulations with literature-based RTM parameters reveals a basin averaged bias of 30 K. Therefore, time series of SMOS TB observations are used to investigate ways for mitigating these large biases. Specifically, the study demonstrates the impact of the LSM soil moisture climatology in the magnitude of TB biases. After CDF matching the SM climatology of the LSM to SMOS retrievals, the average bias decreases from 30 K to less than 5 K. Further improvements can be made through calibration of RTM parameters related to the modeling of surface roughness and vegetation. Consequently, it can be concluded that SM rescaling and RTM optimization are efficient means for mitigating biases and form a necessary preparatory step for data assimilation.

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1. Introduction

The updating of land surface models (LSMs) through remote sensing data assimilation is well-known for its potential to improve hydrologic model predictions (e.g. Pauwels et al. (2001, 2002); Crow and Wood (2003); Reichle et al. (2007); Pan et al. (2009)). Often, the LSMs are updated with observations of the top surface soil moisture (SM) content, since it plays a key role in the partitioning of rainfall into infiltration, runoff, and evapotranspiration. The updating of surface SM may substantially improve the profile SM along, since the errors in surface SM predictions are highly correlated with those at deeper depths (Walker et al. 2001).

The significance of SM observations for hydrologic predictions has fostered the development of remote sensing platforms, such as the Soil Moisture and Ocean Salinity (SMOS) mission (Kerr et al. 2001) and the Soil Moisture Active and Passive (SMAP) mission (Entekhabi et al. 2010), dedicated to observing the dynamics of SM across time and space. These radiometer systems provide indirect estimates of SM, through the close relationship between the observed brightness temperature (TB) emitted by the Earth's surface and the SM content. While it is possible to assimilate the derived SM products, there has been a strong interest in the direct assimilation of satellite-observed TBs (Reichle et al. 2001; Balsamo et al. 2006; Han et al. 2013), since this bypasses the need for ancillary parameters (e.g. surface temperature), and allows for the use of consistent parameters (e.g. soil and vegetation) between the LSM and radiative transfer model (RTM).

The assimilation of TB observations directly requires the use of an RTM as a forward operator, to simulate the top of atmosphere (TOA) TB. However, simulation of unbiased and accurate TBs is far from straightforward due to the complexity of the radiative transfer processes involved (De Lannoy et al. 2013). Furthermore, the parameters in RTMs are typically estimated from local field experiments using ground-based and airborne radiometers (e.g. Sabater et al. (2011); Peischl et al. (2012)), which may not always be appropriate for the simulation of space-borne observations, e.g. by SMOS. Unfortunately, large scale studies

59 on RTM parameterization are hardly available (Drusch et al. 2009; de Rosnay et al. 2009),
 60 and only few studies have used actual SMOS TB data (De Lannoy et al. 2013; Montzka
 61 et al. 2013). Another major difficulty in TB simulation relates to the representation of the
 62 RTM input fields, such as soil temperature, soil moisture, and vegetation parameters, which
 63 are generally obtained from an LSM. Many studies have found large systematic differences
 64 between SM fields modeled through LSMs and those observed by satellite missions (e.g.
 65 Reichle et al. (2004); Gao et al. (2006); Sahoo et al. (2013)). These can be attributed to
 66 several factors (Verhoest et al. 2014), such as approximations and shortcomings in both
 67 the retrieval and land surface models (De Lannoy et al. 2007), and a mismatch in the
 68 vertical representation (Wilker et al. 2006). Radiometer observations are generally sensitive
 69 to only the top few centimeters (Escorihuela et al. 2010), whereas each LSM typically has
 70 its own definition of the top surface layer which is often much thicker than this (Sahoo
 71 et al. 2013). Furthermore, there is often a mismatch in horizontal resolution. Especially for
 72 regional and smaller scale studies, LSMs typically operate at resolutions of 1 to 10 km, whilst
 73 radiometers provide SM at scales of 10 to 40 km (Sahoo et al. 2013). Finally, LSMs may be
 74 optimized toward the simulation of streamflow or land-atmosphere fluxes, rather than SM
 75 representation. For these reasons, LSMs and satellite retrievals generally have different SM
 76 climatologies. Unfortunately, an established consensus on the climatology of SM over large
 77 domains, considering both LSMs and satellite retrievals, is currently lacking (Draper et al.
 78 2013). Nevertheless, when LSM soil moisture is used as input to an RTM, its climatology
 79 has a substantial impact on the magnitude of biases in TB. This becomes evident when
 80 considering the sensitivity of TB to SM, i.e. generally in the order of 2 to 3 K increase per
 81 $0.01 \text{ m}^3 \text{ m}^{-3}$ decrease in SM for low vegetation at around 40° incidence angle (Jackson 1993).

82 In this study, the Community Microwave Emission Modelling (CMEM) platform (Holmes
 83 et al. 2008; Drusch et al. 2009; de Rosnay et al. 2009) is coupled to the Variable Infiltration
 84 Capacity (VIC) LSM (Liang et al. 1994, 1996, 1999) for the simulation of multi-angular and
 85 multi-polarization SMOS TB observations. The TB simulations from this model configu-

86 ration are matched to SMOS observations by calibrating the RTM parameters accordingly.
 87 Previous studies have addressed the global calibration of RTM parameters based on multi-
 88 angular SMOS observations (De Lannoy et al. 2013), and local calibration of temporally
 89 dynamic RTM parameters through data assimilation over a SCAN (Soil Climate Analysis
 90 Network) site in Colorado (Montzka et al. 2013). The novelty of this present study lies in
 91 its focus on the influence of the LSM soil moisture climatology on the TB simulations, the
 92 selection of the RTM calibration parameters, and the dependence of the calibration on the
 93 sensor configuration (— i.e. distinguishing between ascending (A) and descending (D) satel-
 94 lite overpasses and horizontal (H) and vertical (V) polarizations). The study is applied on a
 95 regional scale, covering the Upper Mississippi Basin in the central US. The final aim of this
 96 study is to improve the parameterization of an RTM within a framework that accommodates
 97 for the direct assimilation of multi-angular and multi-polarization TB observations into an
 98 LSM, in order to benefit surface water management.

99 **2. Data and methods**

100 *a. Study site*

101 The Upper Mississippi River Basin is located in central US. The basin covers an area of
 102 about 440000 km², and comprises portions of Minnesota, Wisconsin, Iowa and Illinois. As
 103 can be seen in Figure 1, the land use is primarily agricultural (e.g. corn, soybean, wheat,
 104 etc.), with forests occurring in the Northeast. The basin is characterized by a lack of sig-
 105 nificant topography, which facilitates the retrieval of SM from satellite observations. The
 106 annual precipitation ranges from approximately 475 mm in the North to over 1300 mm in the
 107 South. The southern portion is prone to flooding due to strong summer precipitation, often
 108 enhanced by wet initial conditions. Furthermore, the basin is equipped with an extensive
 109 meteorological network, and is a part of the North American Land Data Assimilation System
 110 (NLDAS) domain (Mitchell et al. 2004). Finally, the catchment is characterized by a low

111 contamination of radio frequency interference (RFI) in the SMOS L-band observations.

112 *b. SMOS observations*

113 SMOS provides regular (± 3 -day repeat period) observations of the TOA TB at global
114 scale, which are operationally used for SM retrieval through the ESA (European Space
115 Agency) Level 2 processor (Kerr et al. 2012). The TB and SM data in this study stem from
116 the Level 3 CATDS (Centre Aval de Traitement des Données SMOS) product (Jacquette
117 et al. 2010). In essence, the Level 3 algorithm is an extension of the Level 2 prototype, em-
118 ploying multi-orbit retrievals of vegetation parameters for the enhancement of SM retrievals
119 over individual orbits.

120 The Level 3 CATDS TB data is a global daily product in full polarization, available
121 in ± 25 km cylindrical projection over the EASE (Equal Area Scalable Earth) grid. Note
122 that the actual resolution of SMOS is ± 43 km. The TB data are transformed from antenna
123 polarization reference (X and Y) to ground reference (H and V) frame, and are angle-binned
124 into fixed angle classes, stretching from 17.5° to 52.5° , with 5° bins. Both ascending and
125 descending data have been extracted over the Upper Mississippi Basin from begin January
126 2010 to end December 2011, with ascending and descending orbits being processed separately.

127 Corresponding Level 3 CATDS ascending and descending SM data are also extracted over
128 the study area from 2010 to 2011 from the 1-day global product. Next to SM, the product
129 also contains quality indices for soil moisture and RFI, as well as science flags indicating the
130 presence of snow, frozen soils, etc. The SMOS data have been extensively filtered, preserving
131 data when soil and air temperatures (according to the LSM forcings and simulations) are
132 larger than 2.5°C , flags for snow and frozen soils (provided by the European Centre for
133 Medium-Range Weather Forecasts) are zero, the probability of RFI is less than 0.2, and
134 fractions of urban and water cover are less than 0.1 (fraction per SMOS cell).

135 *c. The Variable Infiltration Capacity model*

136 The Variable Infiltration Capacity (VIC) model (Liang et al. 1994, 1996, 1999) is a
137 distributed LSM, conserving both the water and energy budgets. During the last decades,
138 the VIC model has been widely-used in a number of applications (e.g. Maurer et al. (2001);
139 Nijssen et al. (2001); Sheffield et al. (2003); Sheffield and Wood (2008)). The grid cell
140 size of VIC can vary from 1 km to hundreds of kilometers, where each cell can be further
141 subdivided into fractions representing specific vegetation types. In this study, the grid
142 spacing corresponds to 0.125° by 0.125° .

143 The simulations make use of the real-time forcing dataset (Cosgrove et al. 2003) prepared
144 for the first and second phase of the NLDAS project (Mitchell et al. 2004). Seven meteo-
145 rological forcing fields were processed at an hourly time step and 0.125° spatial resolution:
146 precipitation, 2-meter air temperature, pressure, vapor pressure, wind speed, and incoming
147 shortwave and longwave radiation. The soil and vegetation parameters employed in VIC
148 were sourced from the NLDAS-1 project, whereas land cover was extracted from the global
149 1-km University of Maryland (UMD) dataset (Hansen et al. 2000). The vegetation leaf area
150 index (LAI) is based on the AVHRR (Advanced Very High Resolution Radiometer) satellite
151 sensor (Gutman and Ignatov 1998). Finally, soil texture was derived from the State Soil Ge-
152 ographic (STATSGO) database (Miller and White 1998), whereas the elevation is described
153 by the global 30 arc-second elevation (GTOPO30) database (Verdin and Greenlee 1996).

154 The model simulations over the Upper Mississippi are performed in full water and energy
155 balance mode, where soil moisture and surface temperature in various layers are simulated
156 on an hourly basis. The number of vertical soil layers has been set to 3, where the first
157 layer represents the top 10 cm of the soil and the second and third layer depths vary between
158 10 cm and 250 cm. Note that this first layer depth may differ from the layer depth observed
159 by SMOS, and may therefore contribute to the occurrence of SM bias between the model
160 simulations and SMOS retrievals. Nevertheless, it was decided not to modify the first layer
161 depth of VIC, as the model employs a one-source energy balance, and consequently depends

on an equivalent surface and vegetation temperature. It should also be remarked that, for this study, the VIC model parameterization was considered to be fixed, having been previously optimized for the purpose of streamflow simulations (Maurer et al. 2002) over the Upper Mississippi Basin.

d. The Community Microwave Emission Modelling platform

The RTM coupled to VIC is the Community Microwave Emission Modelling (CMEM) platform (Holmes et al. 2008; Drusch et al. 2009; de Rosnay et al. 2009) version 4.1. CMEM is used as a forward operator to convert the simulated soil moisture and surface temperatures by VIC into simulations of multi-angular and multi-polarization TOA L-band brightness temperatures $TB_{TOA,p}$ at polarization $p = [H, V]$:

$$TB_{TOA,p} = TB_{au,p} + \exp(-\tau_{atm,p})TB_{TOV,p}, \quad (1)$$

with $TB_{au,p}$ [K] the upward atmospheric contribution, $\tau_{atm,p}$ [–] the atmospheric opacity, and $TB_{TOV,p}$ [K] the TB at top of vegetation (TOV). The latter is calculated through a first-order tau-omega ($\tau - \omega$) model:

$$TB_{TOV,p} = T_{eff} (1 - r_p) \Gamma_p + T_c (1 - \omega_p) (1 - \Gamma_p) (1 + r_p \Gamma_p) + TB_{ad,p} r_p \Gamma_p^2, \quad (2)$$

with T_{eff} [K] the effective temperature of the soil medium, r_p [–] the rough surface reflectivity, Γ_p [–] the vegetation transmissivity, T_c [K] the canopy temperature (set equal to the surface temperature), ω_p [–] the scattering albedo, and $TB_{ad,p}$ [K] the downward atmospheric contribution. The transmissivity of the vegetation can be expressed by:

$$\Gamma_p = \exp\left(-\frac{\tau_{veg,p}}{\cos \theta}\right), \quad (3)$$

with $\tau_{veg,p}$ [–] the optical depth of the standing vegetation and θ [°] the incidence angle.

CMEM has a modular structure, allowing for different parameterization options for the respective contributions from atmosphere, soil, and vegetation. In general, the options selected for this study revert to the L-MEB formulation by Wigneron et al. (2007). The

183 atmospheric contributions ($T_{B_{au,p}}$, $T_{B_{ad,p}}$ and $\tau_{atm,p}$) are described according to Pellarin
 184 et al. (2003). For the soil component, the effective temperature T_{eff} is approximated based
 185 on the surface temperature T_{surf} [K] and the deep-soil temperature T_{deep} [K] as:

$$T_{eff} = T_{deep} + (T_{surf} - T_{deep}) C, \quad (4)$$

186 where the weighting factor C depends on the SM content (Wigneron et al. 2001) by:

$$C = (SM/w_0)^{b_{w_0}}, \quad (5)$$

187 with w_0 and b_{w_0} semi-empirical parameters depending on soil characteristics (mainly soil
 188 texture). As the RTM model is coupled with VIC, the first (0–10 cm) and third (variable
 189 thickness) layer VIC soil temperatures are used to approximate the T_{surf} and T_{deep} , whereas
 190 SM is approximated by the first layer SM from VIC.

191 The rough surface reflectivity parameterization is based on the Q/h formulation by
 192 Choudhury et al. (1979):

$$r_p = (Q R_q + (1 - Q) R_p) \exp(-h \cos^{Nr_p}(\theta)), \quad (6)$$

193 with Q the polarization mixing factor often set to 0 for L-band (Wigneron et al. 2001), q
 194 the opposite polarization of p , h the surface roughness, Nr_p the angular dependence of the
 195 surface roughness, and R_p the smooth surface reflectivity. The latter is given by the Fresnel
 196 equations and is a function of the dielectric constant. The relationship between dielectric
 197 constant and soil moisture is described by Mironov et al. (2004). Finally, the vegetation
 198 optical depth is based on the model by Wigneron et al. (2007), which expresses $\tau_{veg,p}$ as a
 199 function of the optical depth at nadir τ_{NAD} [–]:

$$\tau_{veg,p} = \tau_{NAD} (\cos^2(\theta) t t_p \sin^2(\theta)), \quad (7)$$

200 where $t t_p$ is a parameter accounting for the influence of the incidence angle. The optical
 201 depth at nadir is given by:

$$\tau_{NAD} = b_1 LAI + b_2, \quad (8)$$

202 with b_1 and b_2 being structural vegetation parameters, and LAI the leaf area index.

203 A set of baseline parameter values has been identified, which correspond to the parameter
204 values that are used in the ESA Level 2 processor v5.5.1 (Kerr et al. 2012). The list of
205 parameters is given in Table 1 for each UMD land cover class. Note that for high vegetation
206 types (classes 2 to 7 in Table 1), the annual maximum LAI is used in Equation 8, whereas
207 for low vegetation types (classes 8 to 13 in Table 1), monthly average values (the same as in
208 VIC) are employed.

209 3. CMEM optimization

210 In order to minimize climatological differences between the observed TBs from SMOS
211 and the simulated TBs from the coupled model, a number of RTM parameters are calibrated
212 using multi-angular and multi-polarization SMOS observations. The parameters that are
213 considered for calibration are h , Nr_p , b_1 , b_2 , and τ_p , which were selected based on De Lannoy
214 et al. (2013) and a sensitivity analysis. The b_1 and b_2 coefficients relate the optical thickness
215 of the vegetation to LAI, the h and Nr_p parameters describe the surface roughness and its
216 angular dependence, and τ_p controls the vegetation scattering of microwaves.

217 The following section outlines the calibration procedure and experiments. The calibration
218 is based on SMOS observations and corresponding simulations for the year 2010, whereas
219 data from the year 2011 are used for validation purposes. The calibration will be performed
220 per UMD land cover class (Table 1), except for classes with cover fractions below 1% (such
221 as grasslands), as these may be subject to less accurate parameterization due to under-
222 representation in the calibration dataset. Also water and urban are not included, since the
223 SMOS observations over cells dominated by the latter classes have been filtered.

224 *a. Cal/Val data sets*

225 For each SMOS Level 3 TB observation (including various angle bins and H/V-polarizations)
226 in the 2010 calibration set, 25 EASE grid cells within the Upper Mississippi Basin are ran-
227 domly selected (different grid cells are selected for each observation date). Note that a
228 random selection of cells is performed to limit the size of the calibration data set, while
229 including data from various locations within the basin. For each of the VIC cells that lay
230 within the selected EASE grids (i.e. between 4 and 9 cells), the soil moisture (surface layer),
231 soil temperatures (two layers), sand and clay fractions, and bulk density of VIC are used
232 as input for CMEM. Also used are the VIC land cover types, fractions, and LAI for each
233 VIC sub-grid vegetation layer. Next, CMEM is run for each individual VIC sub-grid vegeta-
234 tion fraction, for both H- and V-polarization and for 8 angle bins from 17.5° to 52.5° (each
235 5°). The simulated TBs are then aggregated to the VIC cell size according to the vegeta-
236 tion fractions within each cell. Finally, the SMOS antenna weight for each VIC grid cell is
237 used to upscale the simulated TBs to the SMOS grid cell. Note that the antenna weighting
238 differs for each cell, as it relies on the SMOS incidence angle, the azimuth angle, and the
239 footprint axis. Thereby, the average of the mean value over each bin is used to compute
240 the weighting function. By repeating the above mentioned steps for each multi-angular and
241 multi-polarization SMOS observation, a calibration data set is established, which conserves
242 the sub-grid vegetation description of the LSM, and comprises data from different incidence
243 angles and polarizations, scattered over the study area. Hereby, independent calibration sets
244 are generated for ascending and descending orbits, to investigate the impact of the overpass
245 on the calibration performance. The same procedure is used for the generation of the val-
246 idation data set based on data from 2011. The ascending and descending calibration and
247 validation data sets each contain in total 8100 data points (TB observations at the SMOS
248 grid) for each polarization. These comprise all 8 angle bins with a frequency of occurrence
249 according to the spatial coverage of the angle bin over each of the randomly chosen cell
250 locations. This implies that inner angles (e.g. 42.5°) are slightly more present than the outer

251 angles (e.g. 17.5° and 52.5°) in the data sets used for calibration and validation.

252 It should be emphasized that the calibration of the RTM in this study is performed per
 253 land cover class instead of on a pixel basis. Pixel-based calibration is difficult to achieve if the
 254 goal is to preserve the sub-grid pixel heterogeneity in terms of vegetation types. Preserving
 255 sub-grid variability in a pixel based calibration would require a high number of parameter
 256 sets for each pixel, which would render the model coupling unfeasible.

257 *b. Calibration algorithm*

258 The calibration is performed using the Particle Swarm Optimization (PSO, Kennedy
 259 and Eberhart (1995)) algorithm. Example applications and details on PSO can be found
 260 in Scheerlinck et al. (2009); Pauwels and De Lannoy (2011). Only a brief explanation and
 261 summary of the selected PSO parameter values are given here. The PSO algorithm iteratively
 262 explores the parameter space and minimizes an a priori defined objective function. The PSO
 263 algorithm modifies a number of parameter sets (or particles) by changing their velocity (speed
 264 and direction) based on the most favorable conditions encountered by an individual particle
 265 and the swarm of particles. Thereby, the modification of individual particles expresses the
 266 cognitive aspect of the optimization algorithm, whereas the modification of the particle
 267 swarm accounts for the social aspect. In this study, the particle swarm size is set to 25,
 268 and the maximum number of iterations to 30. The inertia weight, cognitive and social
 269 parameters are respectively set to 0.7, 0.7, and 1.3. The selected PSO parameter values are
 270 based on De Lannoy et al. (2013), and enforce a stronger social than cognitive effect on the
 271 optimization.

272 The objective function J to be minimized integrates the Kling-Gupta-Efficiency (KGE),
 273 introduced by Gupta et al. (2009), together with a parameter penalty term as:

$$J = W_{\text{KGE}} \frac{1}{N_{\theta,p,o}} \sum_{\theta} \sum_p \sum_o^{\text{H,V A,D}} (1 - \text{KGE}_{\theta,p,o}) + W_{\alpha} \frac{1}{N_{\alpha}} \sum_i^{N_{\alpha}} N_{\alpha} \frac{(\alpha_{0,i} - \alpha_i)^2}{\sigma_{\alpha_{0,i}}^2}, \quad (9)$$

274 with:

$$\text{KGE}_{\theta,p,o} = 1 - \sqrt{W_1 (1 - R_{\theta,p,o})^2 + W_2 (1 - \text{MR}_{\theta,p,o})^2 + W_3 (1 - \text{SR}_{\theta,p,o})^2}, \quad (10)$$

275 where $N_{\theta,p,o}$ is the number of combinations of incidence angle bins θ , polarizations p and
 276 orbits o , while N_α refers to the number of calibrated RTM parameters. W_{KGE} and W_α are
 277 weight-factors for the different penalty terms, respectively set to 100 and 1. The latter
 278 values have been selected to put less constrain on the parameter penalty compared to the
 279 KGE. Further, $\text{KGE}_{\theta,p,o}$ is the KGE for a specific θ , p and o . R is the correlation coefficient,
 280 MR the ratio between the mean of the simulations and the mean of the observations, and
 281 SR the ratio between the standard deviation of the simulations and the standard deviation
 282 of the observations. Note that the latter three criteria should ideally equal to 1, through
 283 which the KGE becomes 1. W_1 to W_3 are weights that can be assigned to specify the relative
 284 importance of the different criteria for the problem at hand. Although different weights have
 285 been tested, the aim of this study is not to perform a thorough optimization of the weights.
 286 Such optimization is a complex task and truly depends on the specific objectives of the
 287 calibration. Therefore, these weights are adopted as an indication of what could be possible.
 288 In this specific study, the weights have been set to $W_1 = 0.05$, $W_2 = 1.95$ and $W_3 = 0$.
 289 The weights W_1 and W_2 were chosen such that emphasis is given to the optimization of the
 290 MR , in order to mitigate biases. W_3 is set to 0, as the improvement in SR comes at the
 291 expense of an increase in bias. Moreover, as the SR simultaneously embeds the variability
 292 of TB in a temporal and spatial context (different grid cells and time steps are contained in
 293 the calibration set), compensating effects, e.g. increasing spatial variability at the expense
 294 of temporal variability needed to be avoided. Hence, SR is arguably less paramount to the
 295 optimization compared to R and MR . Finally, note that the cost function does not account
 296 for uncertainties in the observations, through which the calibration could possibly be prone
 297 to overfitting. However, no clear evidence of overfitting was observed in this study.

298 Besides the KGE, the objective function also minimizes parameter (α_i) deviations from
 299 initial values ($\alpha_{0,i}$) to account for equifinality, i.e. to select a single optimal parameter set

300 from multiple parameter sets that yield a similar KGE. The deviation term is limited by the
 301 variance of a uniform distribution with boundaries $[\alpha_{\min}, \alpha_{\max}]$, given by:

$$\sigma_{\alpha_{0,i}}^2 = \frac{(\alpha_{\max,i} - \alpha_{\min,i})^2}{12}. \quad (11)$$

302 The initial parameter values have been taken from the baseline parameter set given in
 303 Table 1. The boundaries of the different parameters are given in Table 2 and indicate
 304 both the limits of the search area and the expected uncertainty in the prior parameter
 305 estimates. Thereby, it should be noted that Nr_p was not constrained to an initial guess,
 306 i.e. the boundaries on Nr_p are only an indication of the search space limits. The reason
 307 therefore is the large variability of Nr_p observed from experimental data (Wigneron et al.
 308 2001).

309 The restriction to a realistic range of parameter values and the prior penalty term together
 310 preserve a realistic model sensitivity of TB to SM. This sensitivity is generally known to be
 311 an approximate 2–3 K increase in TB for a $0.01 \text{ m}^3 \text{ m}^{-3}$ decrease in soil moisture around 40°
 312 incidence angle for low vegetation (Jackson 1993). As denoted in De Lannoy et al. (2013),
 313 the sensitivity can largely decrease if, for instance, unrealistically high values for roughness
 314 and optical depth are used. In this case, the emission from the soil is very low and thus TB
 315 sensitivity to SM is very low. Such unrealistic parameter values could be obtained due to
 316 compensating effects during the calibration.

317 *c. Calibration experiments*

318 A set of calibration case studies (Table 3) were performed in order to investigate several
 319 aspects in the RTM optimization. A first numerical experiment aims at investigating the
 320 impact of the SM climatology, which is generally characteristic to the LSM, on the TB
 321 simulations with baseline RTM parameters. To this end, a cumulative distribution function
 322 (CDF) matching step was applied to convert the VIC SM output to the climatology of the
 323 SMOS Level 3 SM retrievals. Note that this study refrains from providing recommendations

324 on the optimal SM climatology (e.g. LSM versus SMOS), but rather aims at identifying its
 325 impact in view of RTM optimization for SMOS. The experiment where CDF-matched soil
 326 moisture is used as input to CMEM, without RTM parameter calibration, is referred to as
 327 case 1 in Table 3. The CDFs were computed using the non-parametric kernel-based method
 328 by Li et al. (2010). Thereby, SM values from the year 2010 were used to calculate the CDF
 329 matching coefficients between VIC and SMOS on a pixel-basis, which were subsequently used
 330 to rescale the VIC SM for the year 2011. Figure 2 (a) shows a comparison between the SM
 331 densities from SMOS and VIC before CDF matching, revealing a bias of $0.17 \text{ m}^3 \text{ m}^{-3}$ and
 332 correlation of 0.42. Notably, the VIC SM displays a decreased dynamic range compared to
 333 the SMOS retrievals. Figure 2 (b) shows how the CDF matching reduces the bias to 0.01 m^3
 334 m^{-3} and increases the correlation to 0.75 for the 2011 validation data set.

335 In Table 3, cases 2 to 6 investigate the improvements in TB simulation after calibrating
 336 specific RTM parameters. Given the large impact of roughness on the climatological mean
 337 TB (De Lannoy et al. 2013), the h parameter is included in all cases. Case 2 explores
 338 the calibration of h only, whereas case 3 to 5 simultaneously retrieve Nr , τ , or b_1 and b_2 ,
 339 respectively. Further, case 6 demonstrates the added value of a joint calibration of h , Nr
 340 and τ . Calibration cases 2 to 6 are performed on a data set which includes both ascending
 341 and descending overpasses, as well as both H and V polarizations. Thus, no polarization-
 342 dependent parameters are considered in these cases.

343 Furthermore, cases 7 to 10 are designed to investigate the effect of the radiometer con-
 344 figuration on the calibration. In this context, it is investigated that a differentiation of the
 345 calibration between either polarizations or orbits, or both polarizations and orbits, may en-
 346 hance the performance of the simulations. Finally, case 10 considers the calibration of a
 347 polarization-independent h , and polarization-dependent Nr_p and τ_p parameters, while ac-
 348 counting for ascending and descending orbits separately.

4. Results

a. Baseline run

A baseline run with the RTM parameters of Table 1 was performed to simulate the SMOS TB observations over the Upper Mississippi for the year 2011. Figure 3 shows the basin-averaged angular TB signatures for the (a) ascending and (c) descending orbits, comparing the SMOS observations with the VIC+CMEM simulations. As revealed by this figure, a large bias in the order of 30 K for H-pol and between 27 K (at 17.5°) and 10 K (at 52.5°) for V-pol is found for ascending orbits. Descending orbits are exposed to slightly lower biases of approximately 20 K and 5–15 K for H and V polarization, respectively, which are likely attributed to a lower probability of RFI in descending orbits. Figure 3 moreover displays the RMSE and KGE (with weights $W_1 = 0.05$, $W_2 = 1.95$ and $W_3 = 0$) for each angle and polarization, for (b) ascending and (d) descending orbits. In the case of H-pol, the RMSE increases with incidence angle, whereas the opposite trend is observed for V-pol, irrespective of the orbit. The KGE generally follows a similar behavior, with an increase in performance for lower/higher incidence angles in case of H/V-polarization. Finally, the V-polarized simulations outperform the simulations at H-pol, mostly because of lower biases.

Figure 4 shows the 2011 annual mean (a) SMOS retrievals and (b) simulations of SM over the Upper Mississippi Basin, their (c) bias (SMOS minus VIC) and (d) Spearman rank correlation. The comparison reveals a poor spatial agreement in SM patterns, and large wet model bias that ranges between -5 vol% in the South to -30 vol% in the Northwest. Conversely, the correlation coefficient reaches up to 0.7 for most parts of the basin, demonstrating the agreement in temporal variations between SM simulations and retrievals, particularly in the South and Southwest area that are dominated by low vegetation types (see Figure 1). The correlation results are consistent with comparison studies of SMOS SM products using local measurements (Al Bitar et al. 2012; Leroux et al. 2014). The forest area in the Northeast is mainly characterized by a low temporal correlation close to 0. This

375 may be reasoned by the decreased sensitivity of the SMOS L-band TB observations to SM
376 under dense vegetation cover.

377 Figures 5 and 6 display the 2011 annual mean ascending (a) SMOS TB observations
378 at 42.5° incidence angle, the (b) corresponding VIC+CMEM simulations, their (c) bias
379 and (d) correlation for H- and V-polarization, respectively. Compared to SM, the spatial
380 correspondence between the observations and simulations becomes slightly more prominent,
381 mainly driven by the influences of land cover. The bias is found to be particularly large (up
382 to 50 K) over low vegetated areas at H-pol, whereas biases over forest areas are generally
383 limited within 10 K. These results are consistent with De Lannoy et al. (2013), who found
384 that the use of literature RTM parameters can result in TB biases of 10–50 K against SMOS
385 observations. As for SM, the temporal correlation is especially high in portions dominated
386 with low-vegetation; compared to the SMOS retrievals, the correlations in TB over northern
387 forest areas have increased.

388 *b. Calibration experiments*

389 A set of calibration runs was performed according to Table 3. Table 4 provides an
390 overview of the performance of the different experiments, in comparison to the baseline
391 run during the year 2011. It is important to note that the evaluation criteria in this table
392 are calculated based on datasets combining observations/simulations of different instants in
393 time, spatial locations, and incidence angles. Consequently, regional or seasonal artefacts at
394 specific angle bins are not evaluated by this approach, and will be discussed in Section 4c. In
395 the following, the results of Table 4 are discussed with emphasis on the impact of the LSM
396 SM climatology, the choice of RTM calibration parameters, and the impact of partitioning
397 the calibration between polarizations and orbits.

398 The importance of the SM climatology is evident when comparing the baseline run with
399 case 1. Averaged over orbits and polarizations, the baseline yields a correlation R of 0.67 and
400 RMSE of 29.72 K, with the bias having an absolute value of 20.27 K (the unbiased RMSE

401 (ubRMSE) is thus 21.73 K, given that: $\text{ubRMSE}^2 = \text{RMSE}^2 - \text{bias}^2$). The corresponding
 402 KGE of the baseline equals 0.86. After CDF matching the VIC SM states, the RMSE
 403 decreases to 18.85 K, while bias is reduced to 4.69 K. The unbiased RMSE is also slightly
 404 reduced to 18.26 K. This demonstrates that most of the bias, and a small part of the mismatch
 405 in variability, in the TB simulations is attributed to gross differences in the climatology of
 406 the SM simulations of the LSM against SMOS, with the baseline RTM parameters (Table
 407 1) providing a reasonable simulation of TB once the SM climatology difference has been
 408 accounted for. The impact of SM climatology and the lack of any established consensus
 409 may as well partly explain the large variability in RTM parameters that can be found from
 410 modeling studies in literature (e.g. reviewed in De Lannoy et al. (2013)). In addition to a
 411 decrease in bias and increase in accuracy, the CDF matching improves the correlation to
 412 0.75 as a consequence of the non-linear relationship between TB and SM. Finally, the KGE
 413 is increased from 0.86 to 0.94.

414 Cases 2 to 5 investigate the calibration of h alone, and h in combination with Nr , τ and
 415 b_1 and b_2 , respectively. The results show that none of these calibration experiments are able
 416 to improve the simulations of case 1. This again justifies the use of baseline RTM parameters
 417 as given in Table 1, provided the model SM climatology is corrected. Only for case 6, which
 418 investigates the joint calibration of h , Nr , and τ , is a slight improvement obtained. More
 419 specifically, the RMSE decreases with 1.5 K, with a minor decrease in bias of 0.2 K. These
 420 results are in line with De Lannoy et al. (2013), who observed calibration improvements after
 421 increasing the number of calibration parameters (including h and τ).

422 Given the minor improvements after the joint calibration of h , Nr , and τ , this scenario is
 423 further investigated in cases 7 to 10, where independent calibrations for specific polarizations
 424 and/or orbits are carried out. It shows that separation of polarizations causes a slightly larger
 425 improvement compared to the separation of orbits, whereas treating both polarizations and
 426 orbits separately yields the largest improvement. In the latter case, a decrease of 0.6 K in
 427 RMSE and approximately 1 K in bias was found in comparison with case 6. Finally, case 10

428 indicates that there is no clear need to account for polarization differences in the calibration
429 of h . Hence, the calibration case 10 may be proposed as the most optimal.

430 The improvement after separating ascending (6 am local time) and descending (6 pm local
431 time) orbits may be reasoned by the fact that for ascending orbits, ionospheric effects are
432 expected to be minimal, whereas surface conditions are close to thermal equilibrium. During
433 descending orbits, the temperature gradients can be high (Jackson 1980). Also, the SMOS
434 mission is known to be impacted by RFI (Oliva et al. 2012) and this impact is different
435 for ascending and descending orbits as the instrument is tilted by 32.5° from nadir. The
436 presence of low level RFI in the ascending SMOS observations over Northern America due to
437 the active presence of a military radar system in 2010–2011 was highlighted in Collow et al.
438 (2012) and De Lannoy et al. (2013). Several studies (Bircher et al. 2012; Leroux et al. 2014;
439 Verhoest et al. 2014) have also shown that ascending and descending SMOS data reveal
440 different statistics, supporting the need for different parameterizations. However, a caveat
441 to the differentiation between orbits is the fact that this purposely introduces model bias to
442 match the observation bias. If the objective would be to provide consistent time-independent
443 simulations of TB, a differentiation between orbits may not be advisable. Finally, the use
444 of polarization-dependent surface roughness and (particularly) vegetation parameters may
445 be justified by differences in radiative transfer between polarizations as implemented in the
446 L-MEB model (Wigneron et al. 2001) and validated using local radiometer and SMOS data
447 (Wigneron et al. 2012).

448 *c. Validation of calibration case 10*

449 The calibrated parameters associated with case 10 are further used in a coupled VIC+CMEM
450 model simulation over the Upper Mississippi for 2011. Table 5 shows the parameters ob-
451 tained for ascending and descending orbits for each land cover class with cover fraction
452 larger than 1%, except for water and urban. The roughness h of low vegetation types (e.g.
453 wooded grassland and cropland) slightly increased, mainly for ascending orbits. The single-

454 scattering albedo τ_p remained close to the baseline for ascending orbits, whereas a slight
 455 increase is observed for descending orbits. Furthermore, values for low vegetation are found
 456 to be larger than zero for all polarizations and orbits. Finally, large differences are occur-
 457 ring in Nr_p even within classes of low and high vegetation types as this parameter was not
 458 constrained towards the initial parameter values. Nevertheless, the H-pol results may indi-
 459 cate a sub-optimal performance of the initial value (equal to 2 for all vegetation types), as
 460 calibrated values are mostly in the range of $[0, 1]$. For V-pol, it is less clear to which values
 461 the calibration is converging.

462 To demonstrate the improvements made with respect to the baseline, Figure 7 shows the
 463 angular signature for the 2011 validation data set. In comparison with Figure 3, it clearly
 464 shows a reduction in bias (< 10 K) over all angle bins. Furthermore, the RMSE decreases
 465 significantly to less than 20 K in all cases, whereas the KGE increases to above 0.9. Finally,
 466 after the RTM optimization, the TB simulations show a comparable accuracy (RMSE, KGE)
 467 over all angles, which was not the case for the baseline simulations (see Figure 3).

468 Figures 8 and 9 show a comparison between the simulations and observations of the mean
 469 2011 ascending TB at 42.5° incidence angle, after SM CDF matching and RTM calibration,
 470 for H- and V-polarization respectively. Although the basin average TB bias remains well
 471 below 5 K, considerable regional biases are still encountered. Particularly for H-polarization,
 472 the simulated TBs in the Northwest show a warm model bias compared to the SMOS obser-
 473 vations, whereas the opposite is true in the Southwest. Since large parts of these two regions
 474 share the same dominant land cover type (i.e. cropland), whilst the soil moisture bias has
 475 been almost completely removed through CDF matching, the remaining cause for the ob-
 476 served systematic differences can be found in measurement errors, systematic forcing errors
 477 (e.g. precipitation), or the characterization of the vegetation. Specifically for vegetation, the
 478 Level 3 SMOS retrievals employ static land use maps from ECOCLIMAP and related LAI.
 479 Based on this information, the optical thickness of the vegetation is dynamically retrieved
 480 in conjunction with soil moisture (Kerr et al. 2012). In the case of VIC, the land cover

481 is sourced from the UMD, with fixed monthly LAI parameters based on AVHRR satellite
 482 data. Consequently, regional differences in vegetation characterization may cause biases in
 483 TB, notwithstanding the unbiased soil moisture fields. Further removal of the regional bias
 484 would require pixel-based RTM calibration, or post-processing, e.g. through CDF matching
 485 of the TB simulations or observations. However, it should be recalled that the present study
 486 does not apply pixel-based calibration in order to preserve the sub-grid vegetation variabil-
 487 ity of VIC and simplify the coupling with the RTM. Finally, the Spearman rank correlation
 488 between the observations and simulations of TB is found to be particularly high over low
 489 vegetation, with R-values up to 0.9. Moreover, the correlation has increased after applying
 490 the SM CDF matching, as seasonal TB discrepancies have been reduced through adjusting
 491 SM which non-linearly relates to TB.

492 Figure 10 displays maps of R, MR, SR, and KGE, averaged over all angle bins, polar-
 493 izations and orbits. In this case, the KGE has been calculated with weights (W_1 to W_3)
 494 equal to 1. The choice of equal weights is motivated by the fact that SR is considered a
 495 valuable criterion for pixel-based evaluation; no compensating effects can occur, e.g. due
 496 to the embedding of spatial variability as in the calibration objective function. Again, the
 497 correlation coefficients are high over areas dominated by low vegetation, whereas slightly
 498 lower correlations are found in forest areas mainly in the North. The bias is low over most
 499 parts, however, a warm model bias (ratio of simulations over observations) is found in the
 500 North-western cropland area, whereas a cold bias is observed in the South, dominated by
 501 cropland and wooded grassland. The ratio of the standard deviation shows a large contrast
 502 between low and high vegetation. While SR is close to one for low vegetation, a large un-
 503 derestimation of the TB variability is observed over forests. This may arguably be related
 504 to shortcomings of the model in the characterization of the surface emission and penetration
 505 depth over forest areas. As can be seen in Figure 10 (d), the KGE is mainly influenced
 506 by R and SR, showing lower efficiencies in the forested Northeast. Nevertheless, the KGE
 507 demonstrates the ability for accurately simulating TBs over low vegetation, with efficiencies

508 between 0.6 and 0.8.

509 Finally, time series for 2011 of simulated and observed TB are shown in Figure 11, for
510 ascending orbits at 42.5° , at H- and V-polarization. The time series have been obtained for
511 a SMOS pixel (lat = 42.8260° , lon = -91.1060°) covered for 82% by forest types and another
512 pixel (lat = 40.2180° , lon = -88.5030°) covered for 95% by cropland. As was also revealed
513 by Figure 10, the forest simulations lack the temporal variability observed by SMOS, al-
514 though seasonal patterns are captured well. Also, some of the SMOS observations might
515 still be affected by errors such as those caused by RFI (e.g. the high TB-H observation at
516 DOY 150). A slight overestimation by VIC+CMEM is still observed in winter months for
517 H-polarization, whereas summer TBs are slightly underestimated at V-polarization. Nev-
518 ertheless, it should be noted that this figure provides an example for only one forest pixel.
519 Hence, findings for this specific location are not necessarily true for other pixels dominated
520 by forest cover. Over cropland, the simulations at both H- and V-polarization generally
521 show a good correspondence with the SMOS observations. In this case, observations and
522 simulations are characterized by high correlation and low bias, while exposing similar levels
523 of variability.

524 5. Conclusions

525 To facilitate the direct assimilation of multi-angular/polarization SMOS TB observations,
526 the Community Microwave Emission Modelling platform (CMEM) was coupled to the VIC
527 land surface model. Such direct assimilation of TB observations can be of high value in
528 time-constrained forecasting applications, e.g. of hydrologic events, as it circumvents the
529 need for SM retrieval data that are generally provided with longer time-lag. However, the
530 coupling of an LSM with RTM poses significant challenges when the objective is to simulate
531 accurate and un-biased TBs in comparison with SMOS observations. This study shows
532 that propagation of the VIC soil moisture and surface temperature fields through CMEM,

533 using literature-based RTM parameters, may cause biases in TB that locally reach up to
534 50 K, with an average of about 30 K. A number of experiments were conducted in order to
535 mitigate biases and improve the accuracy of the simulations.

536 The VIC SM is found to show mean annual discrepancies with the corresponding SMOS
537 retrievals in the range of 10 to 30 vol%. Hence, optimization of the RTM using the direct SM
538 output from VIC may lead to parameter combinations that decrease the sensitivity of TB to
539 SM, thus motivating the rescaling of VIC SM. After rescaling the VIC SM to the climatology
540 of SMOS through CDF matching, the average TB bias reduced to less than 5 K, even with
541 literature-based RTM parameterization. In addition to mitigating biases, the CDF matching
542 of SM also increased the temporal correlation between the TB observations and simulations,
543 as a result of the non-linear relation of TB to SM. This demonstrates that the literature
544 parameters, which are also employed in the operational SMOS retrieval algorithm, provide
545 a realistic characterization of the surface and vegetation. Furthermore, it shows that in the
546 case of L-band brightness temperature assimilation, some bias correction to the LSM SM
547 state may be needed.

548 Through a series of RTM calibration experiments, optimal calibration parameters and
549 associated RTM parameter values were selected for each land cover class present in the
550 Upper Mississippi Basin. The calibration of surface roughness h alone, or in combination
551 with either the angular dependence, Nr , the scattering albedo, τ , or the vegetation optical
552 depth (b_1 and b_2) parameters, did not further improve the performance of the simulations.
553 Only a combination of three calibration parameters, i.e., h , Nr and τ , slightly decreased
554 the RMSE (17.36 K) and bias (4.48 K) of the TB simulations. Further improvements in
555 RMSE (16.68 K) and bias (3.79 K) were achieved by separating the calibration for H- and
556 V-polarization, and ascending and descending orbits.

557 A spatio-temporal analysis of the optimized TB simulations over the Upper Mississippi
558 Basin revealed that regional biases (up to 20 K) are still unresolved, particularly in the North-
559 western cropland area, and wooded grassland area in the South. This may be attributed to

560 differences in the characterization of vegetation between the LSM and the SMOS retrieval
561 algorithm. However, most other areas were characterized by low bias (<5 K). Finally, the
562 simulations over forest were found to lack the variability observed by SMOS over short
563 time scales. In combination with lower temporal correlations, forest areas were therefore
564 characterized by lower values of the KGE, which is a combined measure for correlation, bias
565 and variability. For most cropland and low vegetation areas, the coupled model was found
566 to provide accurate and unbiased TB simulations, characterized by KGE values of 0.6 to 0.8,
567 which is a prerequisite for the assimilation of SMOS TB observations to benefit hydrologic
568 applications.

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TABLE 1. The baseline RTM parameters for the UMD land cover types.

ID	UMD land cover	Cover [%]	b_1	b_2	Nr_H	Nr_V	tt_H	tt_V	h	τ_H	τ_V
1	Water	1.81	0	0	0	0	0	0	0	0	0
2	Evergreen needleleaf	1.64	0.36	0	2	0	1	1	0.3	0.08	0.08
3	Evergreen broadleaf	0	0.29	0	2	0	1	1	0.3	0.08	0.08
4	Deciduous needleleaf	0	0.36	0	2	0	1	1	0.3	0.08	0.08
5	Deciduous broadleaf	12.93	0.29	0	2	0	1	1	0.3	0.08	0.08
6	Mixed forest	6.61	0.325	0	2	0	1	1	0.3	0.08	0.08
7	Woodland	14.17	0.29	0.03	2	0	1	1	0.3	0.08	0.08
8	Wooded grassland	18.67	0.06	0	2	0	1	1	0.1	0	0
9	Closed shrubland	0	0.06	0	2	0	1	1	0.1	0	0
10	Open shrubland	0	0.06	0	2	0	1	1	0.1	0	0
11	Grassland	0.44	0.06	0	2	0	1	1	0.1	0	0
12	Cropland	42.32	0.06	0	2	0	1	1	0.1	0	0
13	Bare ground	0	0.06	0	2	0	1	1	0.1	0	0
14	Urban and built	1.41	0	0	1	1	0	0	0	0	0

TABLE 2. RTM calibration parameters and selected boundaries.

Parameter	Min	Max
h	0	2
Nr_p	-1	2
τ_p	0	0.2
b_1	0	0.7
b_2	0	0.7

TABLE 3. RTM calibration cases.

Case	Orbits	Polarizations	SM CDF	h	Nr	τ	b_1 and b_2
Baseline	A and D	H and V	No	—	—	—	—
Case 1	A and D	H and V	Yes	—	—	—	—
Case 2	A and D	H and V	Yes	X	—	—	—
Case 3	A and D	H and V	Yes	X	X	—	—
Case 4	A and D	H and V	Yes	X	—	X	—
Case 5	A and D	H and V	Yes	X	—	—	X
Case 6	A and D	H and V	Yes	X	X	X	—
Case 7	A and D	H or V	Yes	X	X	X	—
Case 8	A or D	H and V	Yes	X	X	X	—
Case 9	A or D	H or V	Yes	X	X	X	—
Case 10	A or D	H and/or V	Yes	X	X	X	—

TABLE 4. Evaluation of the calibration experiments based on the 2011 validation data set.

		Baseline	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9	Case 10
A-H	RMSE [K]	40.68	22.03	21.05	19.93	20.72	20.32	19.18	18.95	18.62	18.26	18.10
	Bias [K]	32.43	5.50	3.90	1.92	4.39	1.97	2.05	0.95	-1.79	-2.99	-2.85
	R [-]	0.67	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.77	0.77	0.76
	KGE [-]	0.79	0.94	0.94	0.95	0.94	0.94	0.95	0.95	0.95	0.94	0.94
A-V	RMSE [K]	24.52	14.25	14.06	14.11	13.72	14.42	13.68	13.97	13.85	13.93	13.66
	Bias [K]	18.75	-3.20	-4.52	-3.58	-3.94	-4.60	-2.53	-1.44	-5.69	-4.07	-4.48
	R [-]	0.70	0.78	0.78	0.78	0.78	0.79	0.78	0.78	0.79	0.79	0.78
	KGE [-]	0.88	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.94	0.95	0.95
D-H	RMSE [K]	33.92	21.26	20.78	20.29	20.15	20.48	19.46	19.63	18.93	18.49	18.96
	Bias [K]	21.30	-0.86	-2.71	-4.89	-2.09	-4.58	-4.73	-5.85	-1.66	-2.63	-2.46
	R [-]	0.63	0.74	0.74	0.74	0.75	0.74	0.75	0.75	0.75	0.75	0.75
	KGE [-]	0.85	0.94	0.94	0.94	0.94	0.94	0.94	0.93	0.94	0.94	0.94
D-V	RMSE [K]	19.77	17.85	18.28	17.89	17.70	18.53	17.14	16.83	16.39	16.29	15.99
	Bias [K]	8.58	-9.20	-10.76	-9.69	-10.05	-10.65	-8.59	-7.18	-6.36	-4.62	-5.39
	R [-]	0.67	0.73	0.74	0.73	0.74	0.74	0.73	0.73	0.73	0.73	0.72
	KGE [-]	0.91	0.92	0.92	0.92	0.92	0.92	0.92	0.93	0.93	0.93	0.93
Mean	RMSE [K]	29.72	18.85	18.54	18.06	18.07	18.44	17.36	17.34	16.95	16.74	16.68
	Bias [K]	20.27	4.69	5.47	5.02	5.12	5.45	4.48	3.85	3.87	3.58	3.79
	R [-]	0.67	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.75
	KGE [-]	0.86	0.94	0.94	0.94	0.94	0.94	0.94	0.94	0.94	0.94	0.94

TABLE 5. The calibrated RTM parameters of case 10 for the UMD land cover types.

ID	UMD land cover	Ascending					Descending				
		h	Nr_H	Nr_V	τ_H	τ_V	h	Nr_H	Nr_V	τ_H	τ_V
2	Evergreen needleleaf	0.32	0.85	0.65	0.04	0.12	0.29	0.35	0	0.16	0.11
5	Deciduous broadleaf	0.13	0.48	-0.88	0.07	0.05	0.47	1.67	1.08	0.12	0.13
6	Mixed forest	0.47	0.64	1.19	0.04	0.07	0.33	1.49	0.8	0.15	0.15
7	Woodland	0.09	0.53	0.63	0.09	0.09	0.41	0.62	-0.8	0.11	0.14
8	Wooded grassland	0.29	0.35	1.35	0.01	0.07	0.22	-0.5	0.95	0.05	0.11
12	Cropland	0.26	-0.34	2	0.04	0.03	0.15	1.22	2	0	0.03

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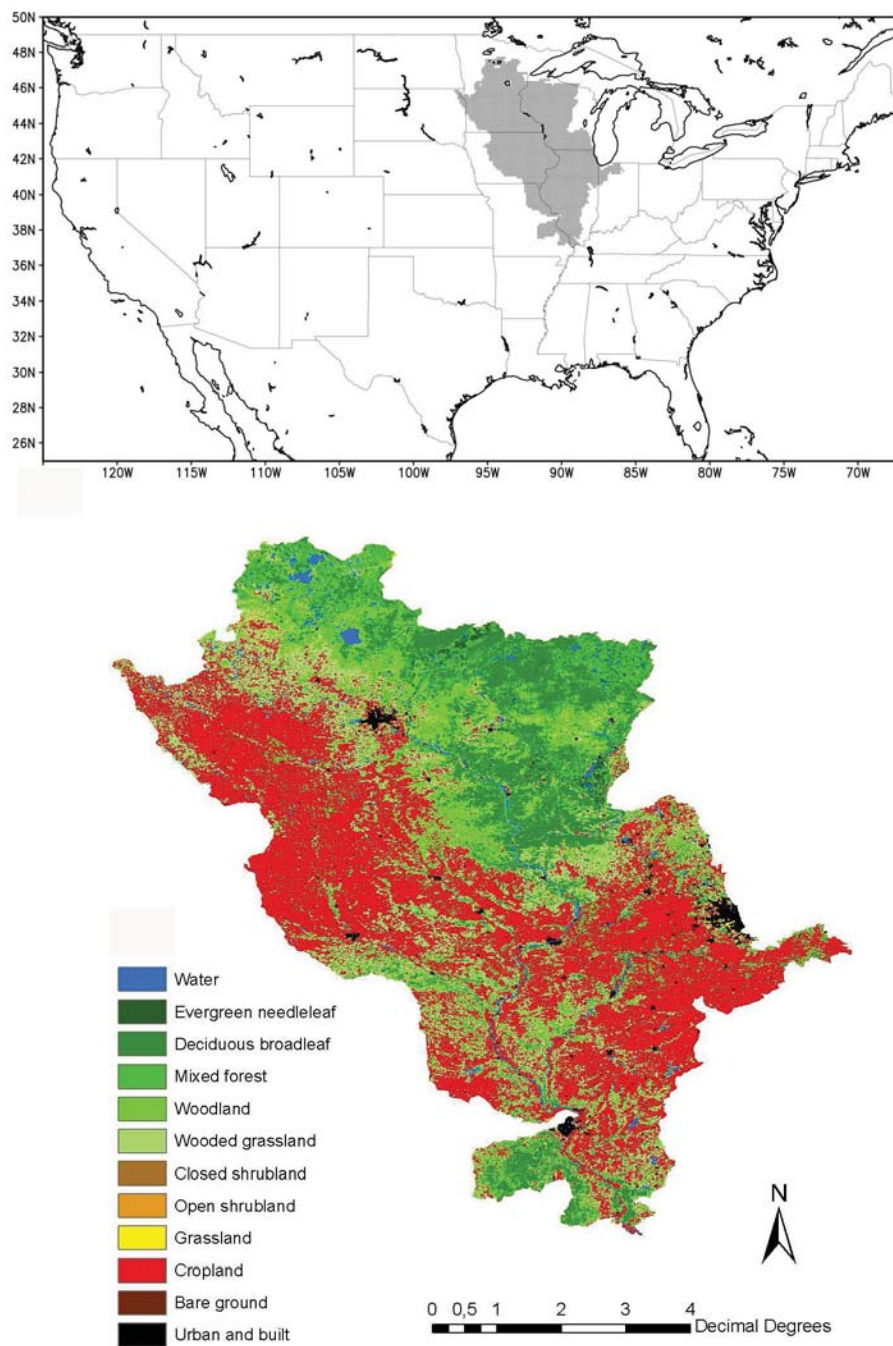


FIG. 1. Land cover map of the Upper Mississippi River basin, following the University of Maryland (UMD) classification (Hansen et al. 2000).

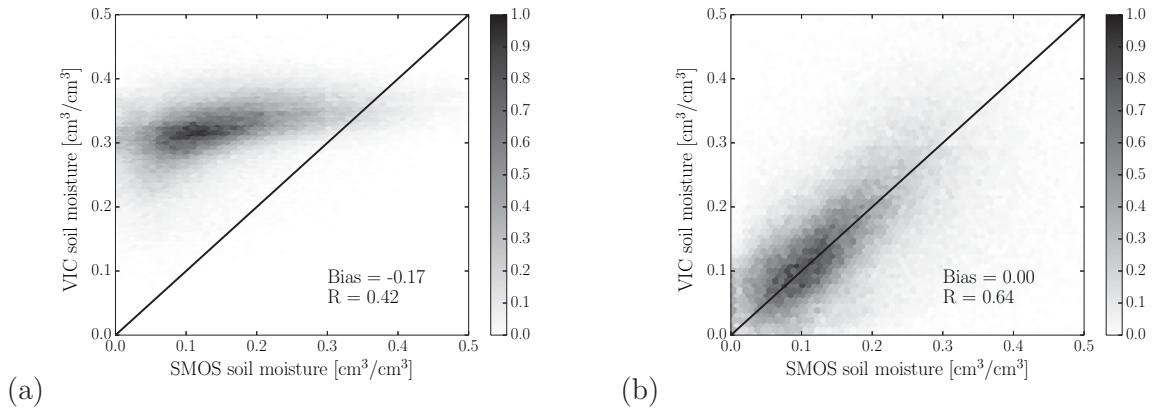


FIG. 2. Density scatter plots between 2011 VIC and SMOS soil moisture [vol%] (a) prior to and (b) after CDF matching.

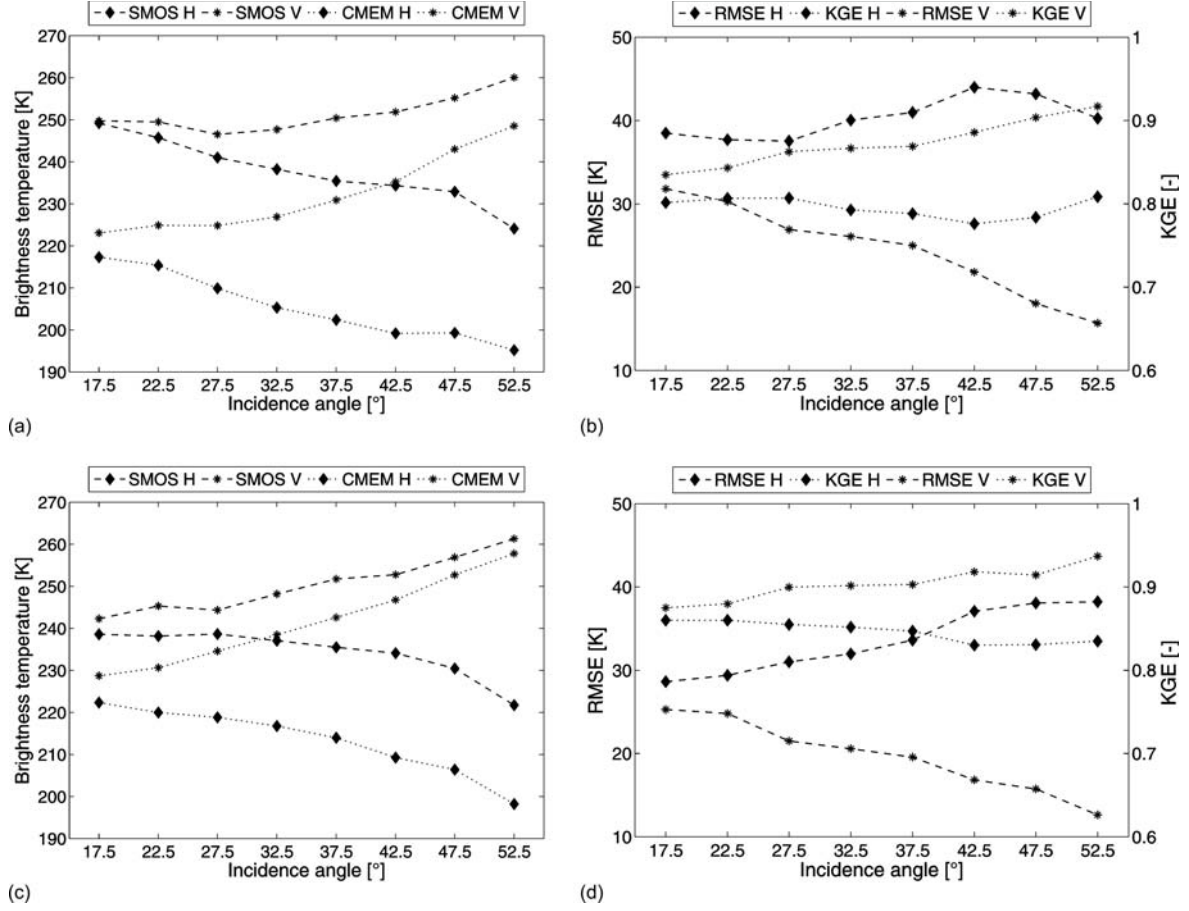


FIG. 3. The basin averaged angular TB [K] signatures of the SMOS observations and baseline VIC+CMEM simulations for 2011, along with the RMSE [K] and KGE [-] for (a, b) ascending and (c, d) descending orbits, respectively.

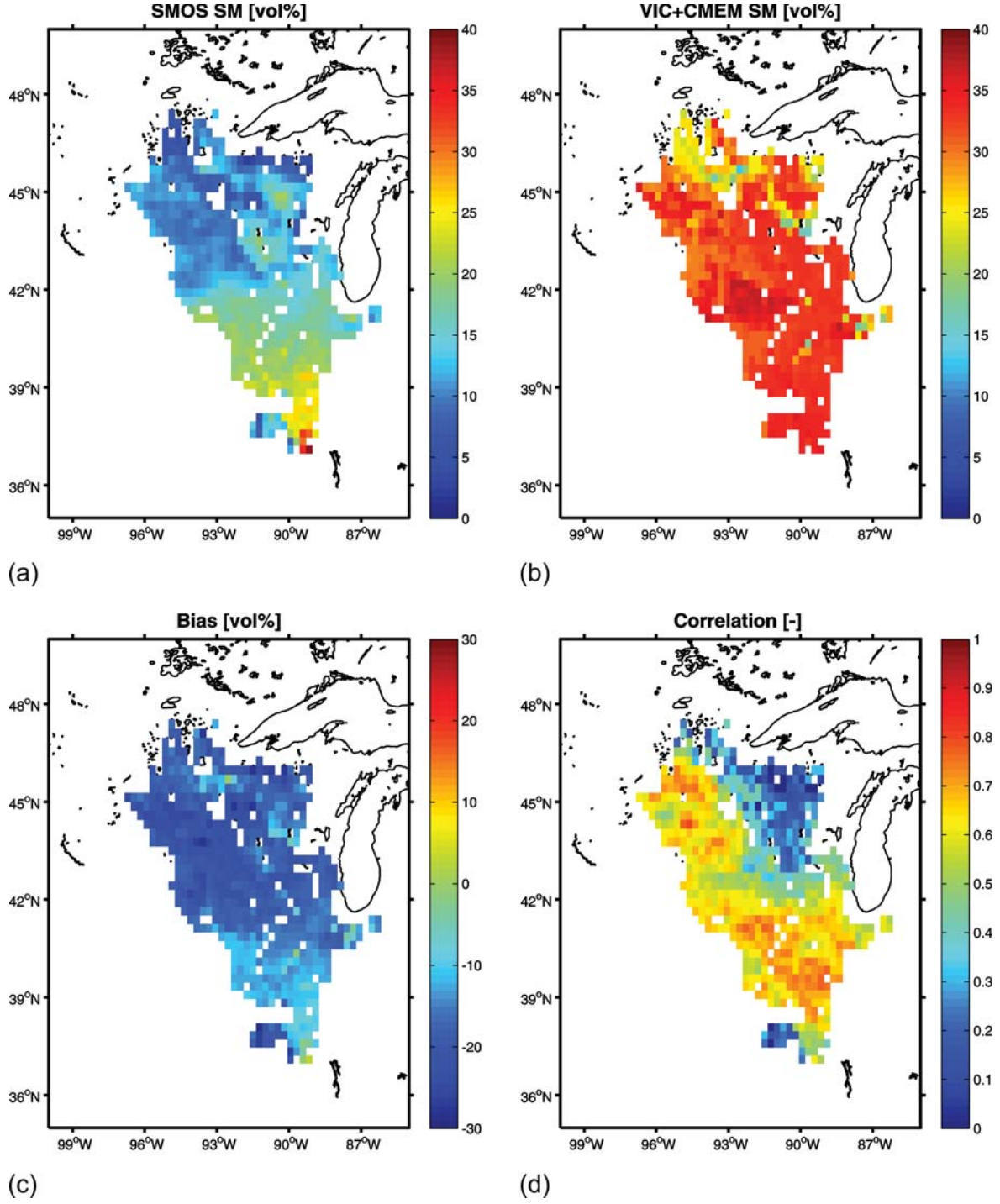


FIG. 4. The 2011 annual mean ascending SM [vol%] (a) retrieved from SMOS and (b) simulated by VIC, along with the corresponding (c) bias [vol%] (SMOS minus model) and (d) Spearman rank correlation [-].

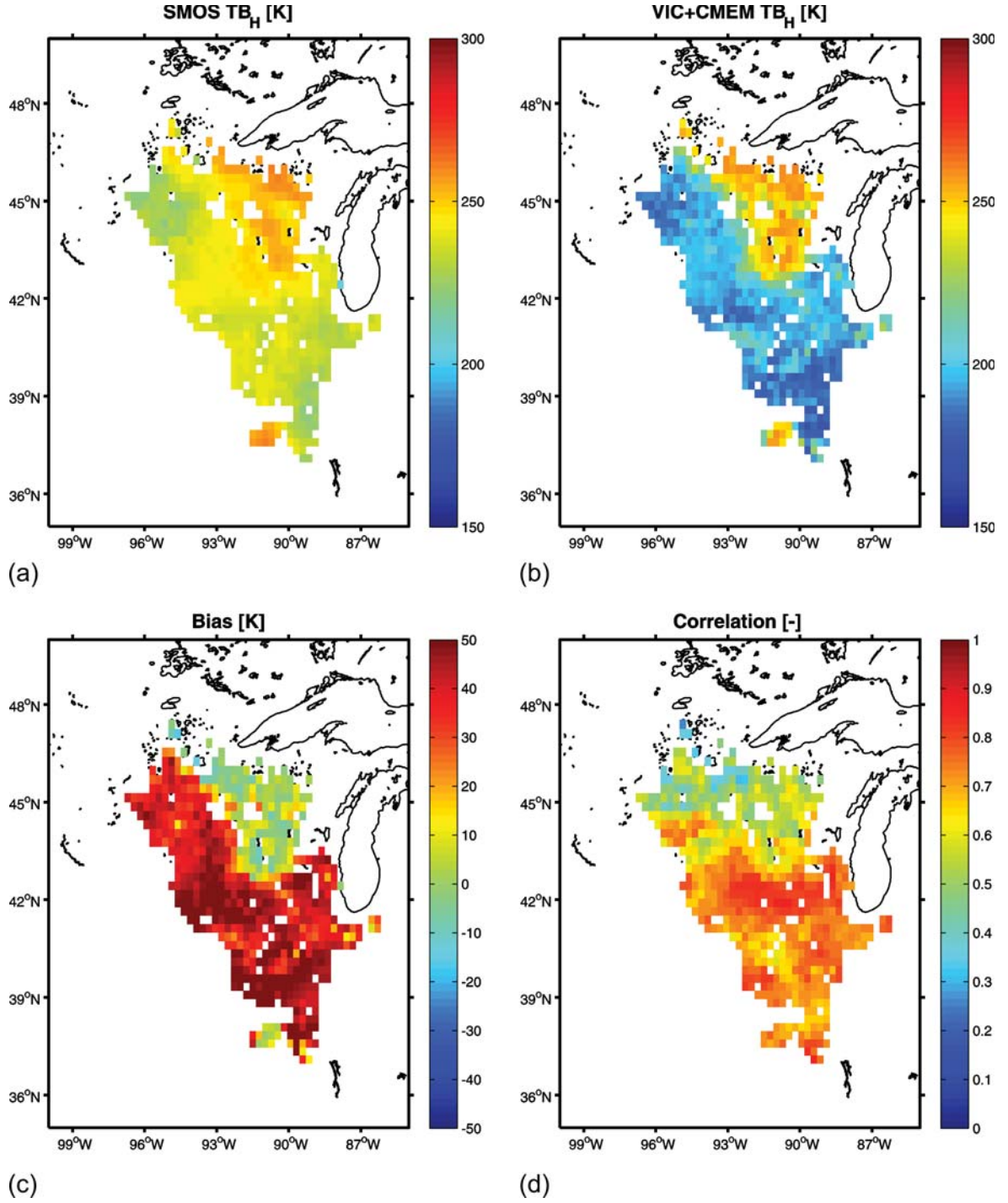


FIG. 5. The 2011 annual mean ascending TB_H [K] at 42.5° (a) observed by SMOS and (b) simulated by the baseline VIC+CMEM, along with the corresponding (c) bias [K] (SMOS minus model) and (d) Spearman rank correlation [-].

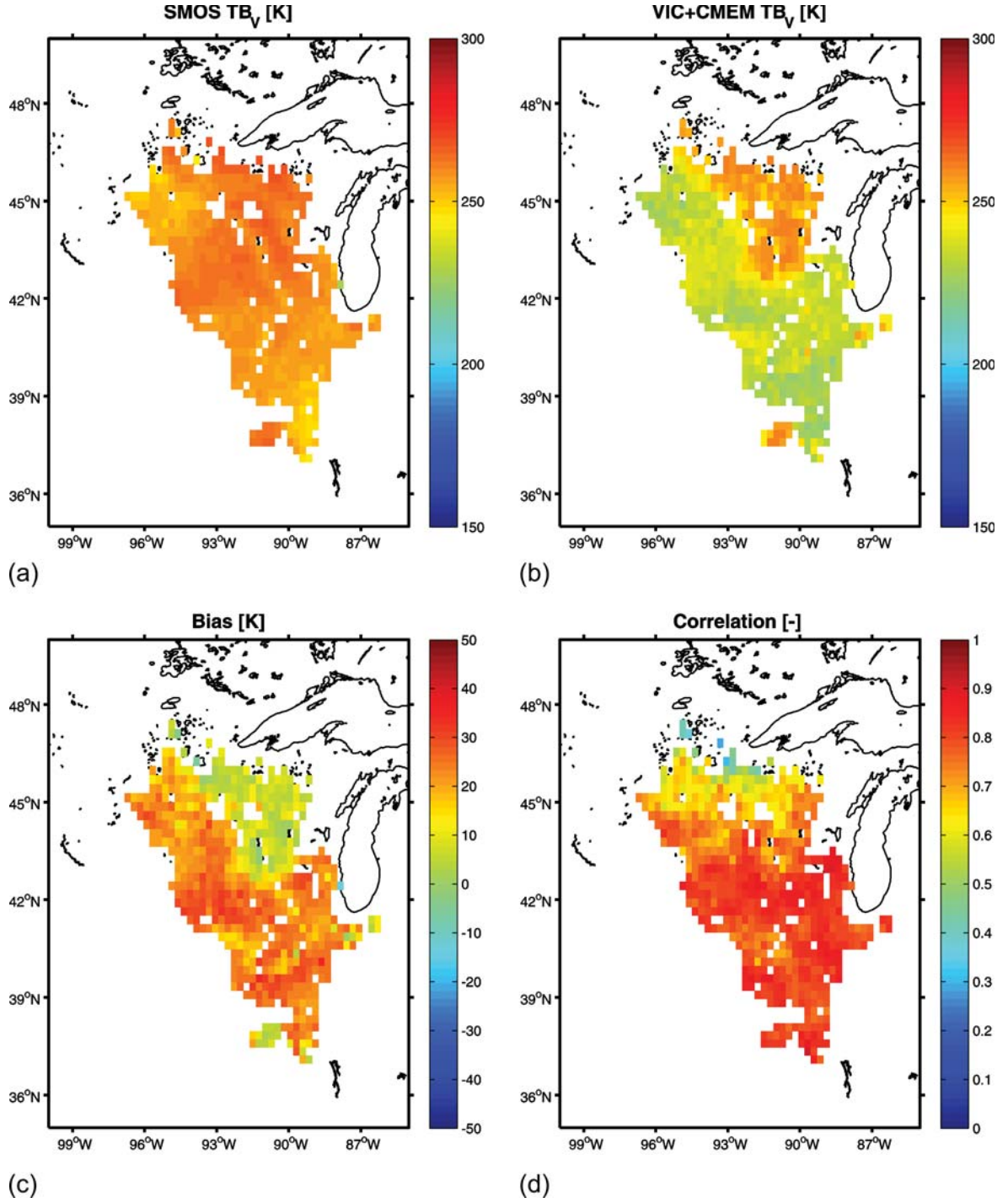


FIG. 6. The 2011 annual mean ascending TB_v [K] at 42.5° (a) observed by SMOS and (b) simulated by the baseline VIC+CMEM, along with the corresponding (c) bias [K] (SMOS minus model) and (d) Spearman rank correlation [-].

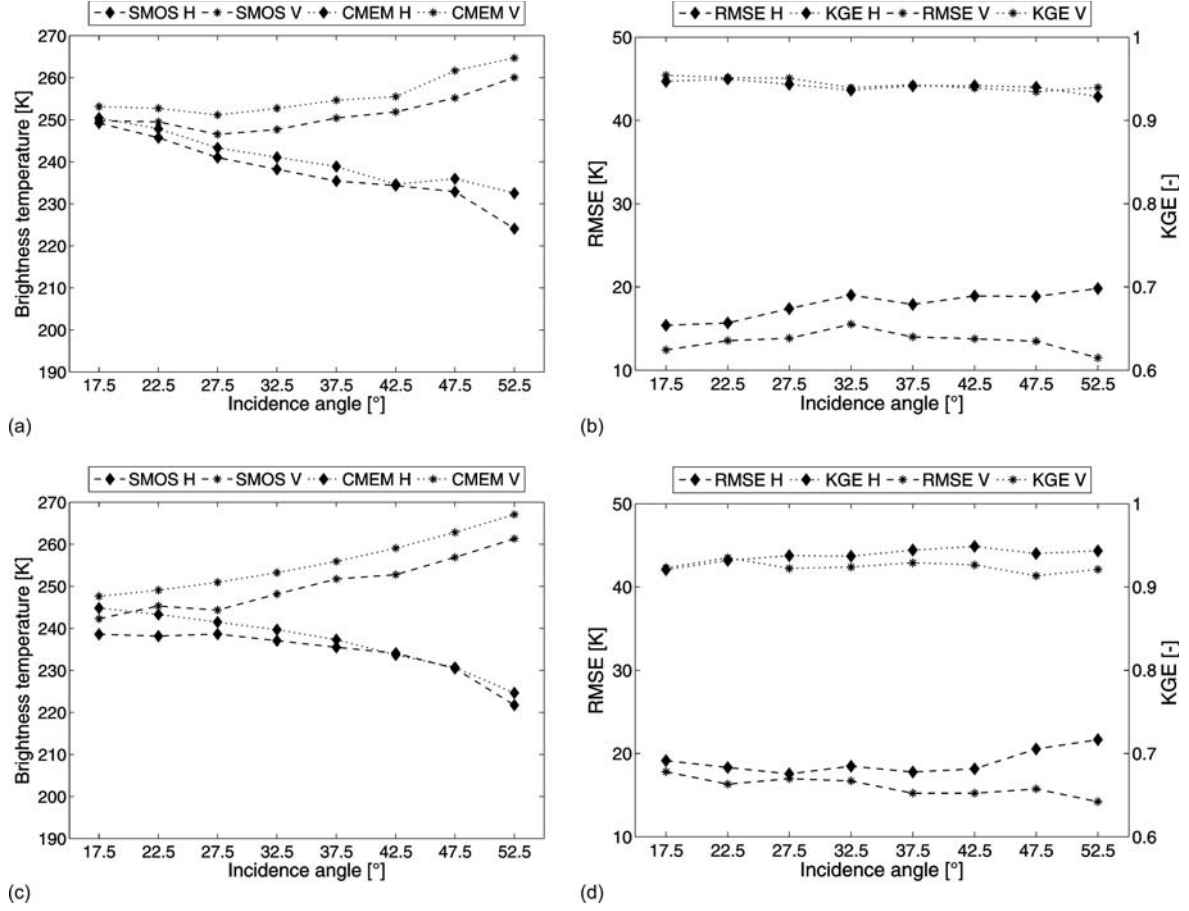


FIG. 7. The basin averaged angular TB [K] signatures of the SMOS observations and calibrated (case 10) VIC+CMEM simulations for 2011, along with the RMSE [K] and KGE [-] for (a, b) ascending and (c, d) descending orbits, respectively.

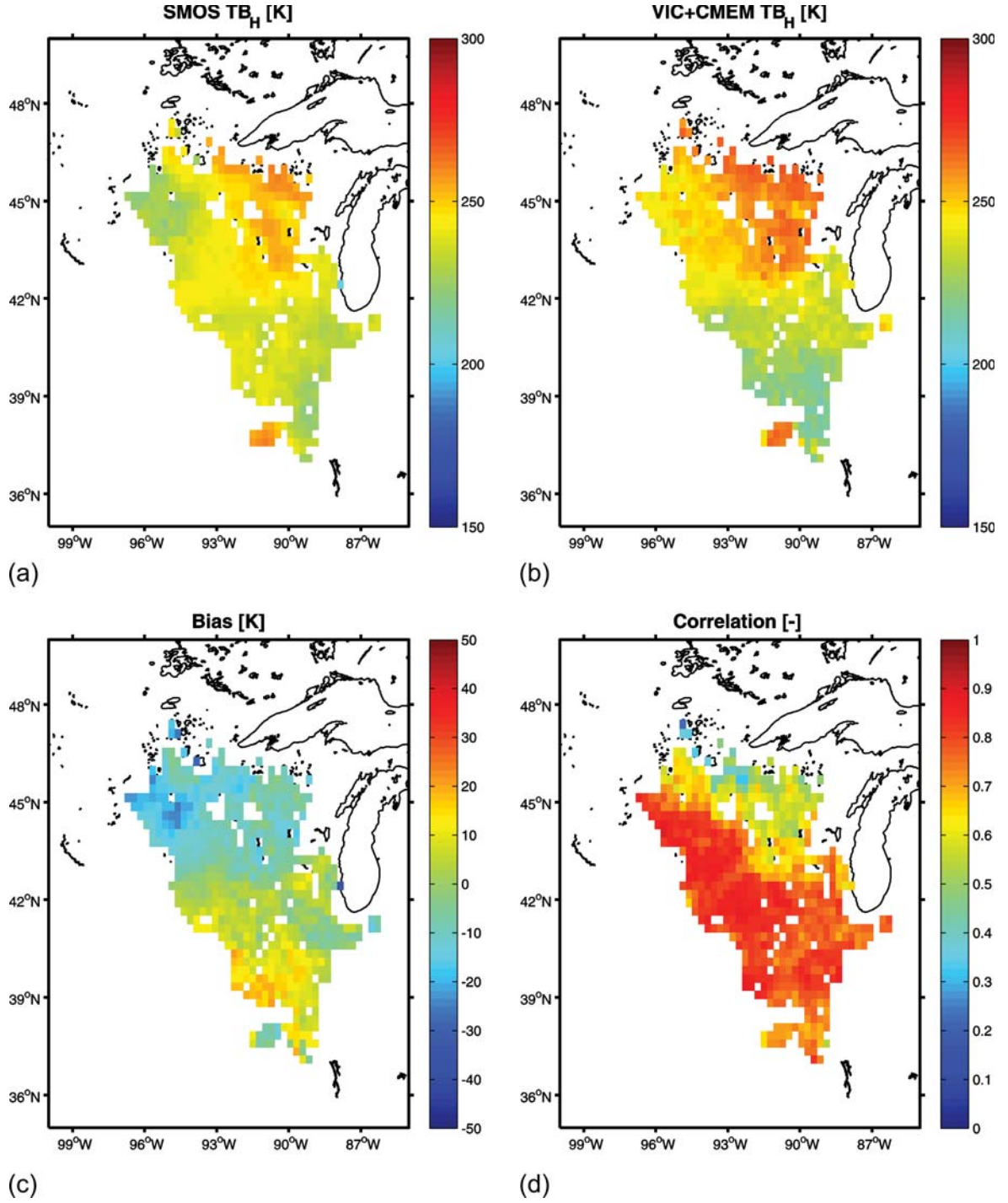


FIG. 8. The 2011 annual mean ascending TB_H [K] at 42.5° (a) observed by SMOS and (b) simulated by the calibrated (case 10) VIC+CMEM, along with the corresponding (c) bias [K] (SMOS minus model) and (d) Spearman rank correlation [-].

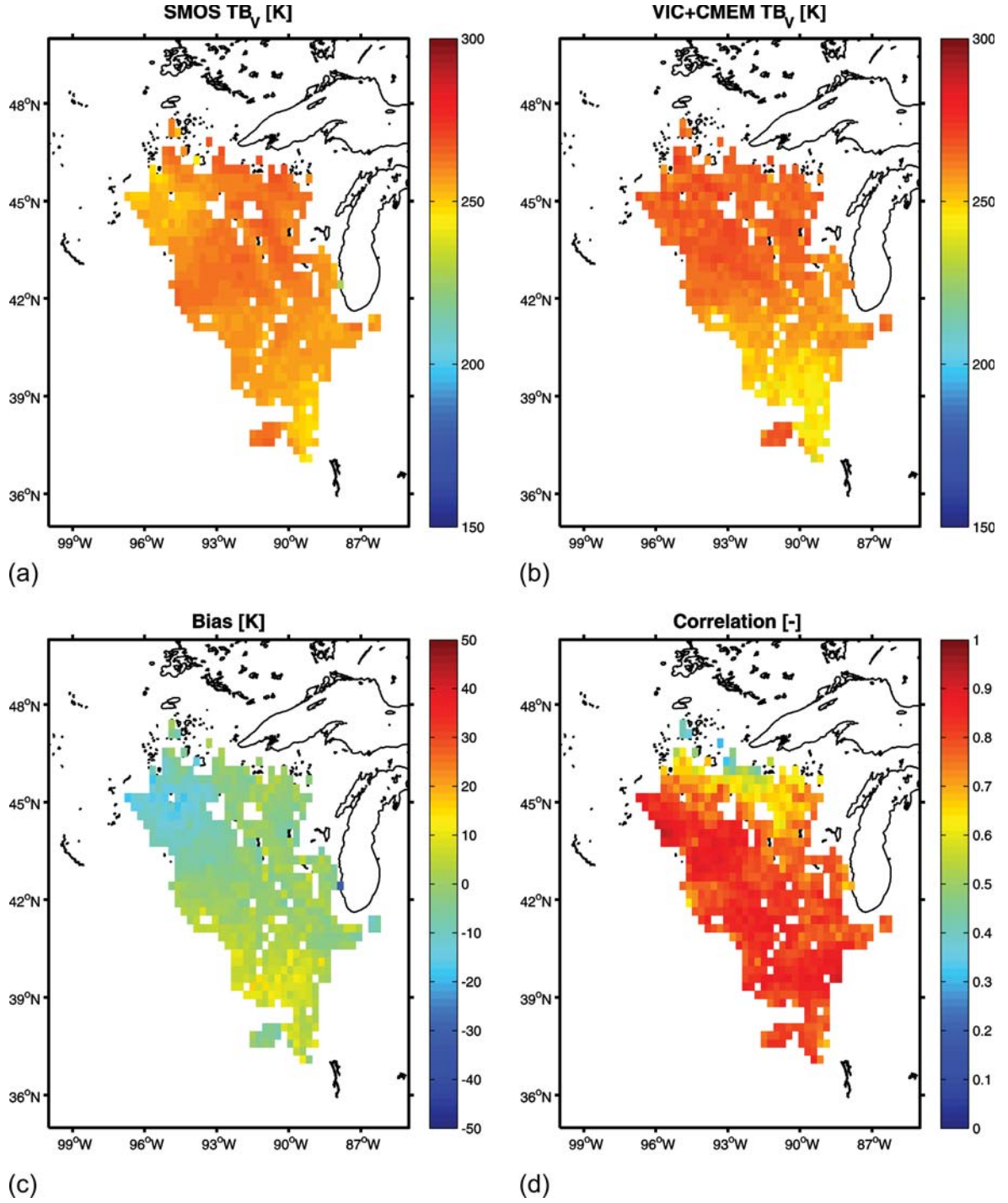


FIG. 9. The 2011 annual mean ascending TB_v [K] at 42.5° (a) observed by SMOS and (b) simulated by the calibrated (case 10) VIC+CMEM, along with the corresponding (c) bias [K] (SMOS minus model) and (d) Spearman rank correlation [-].

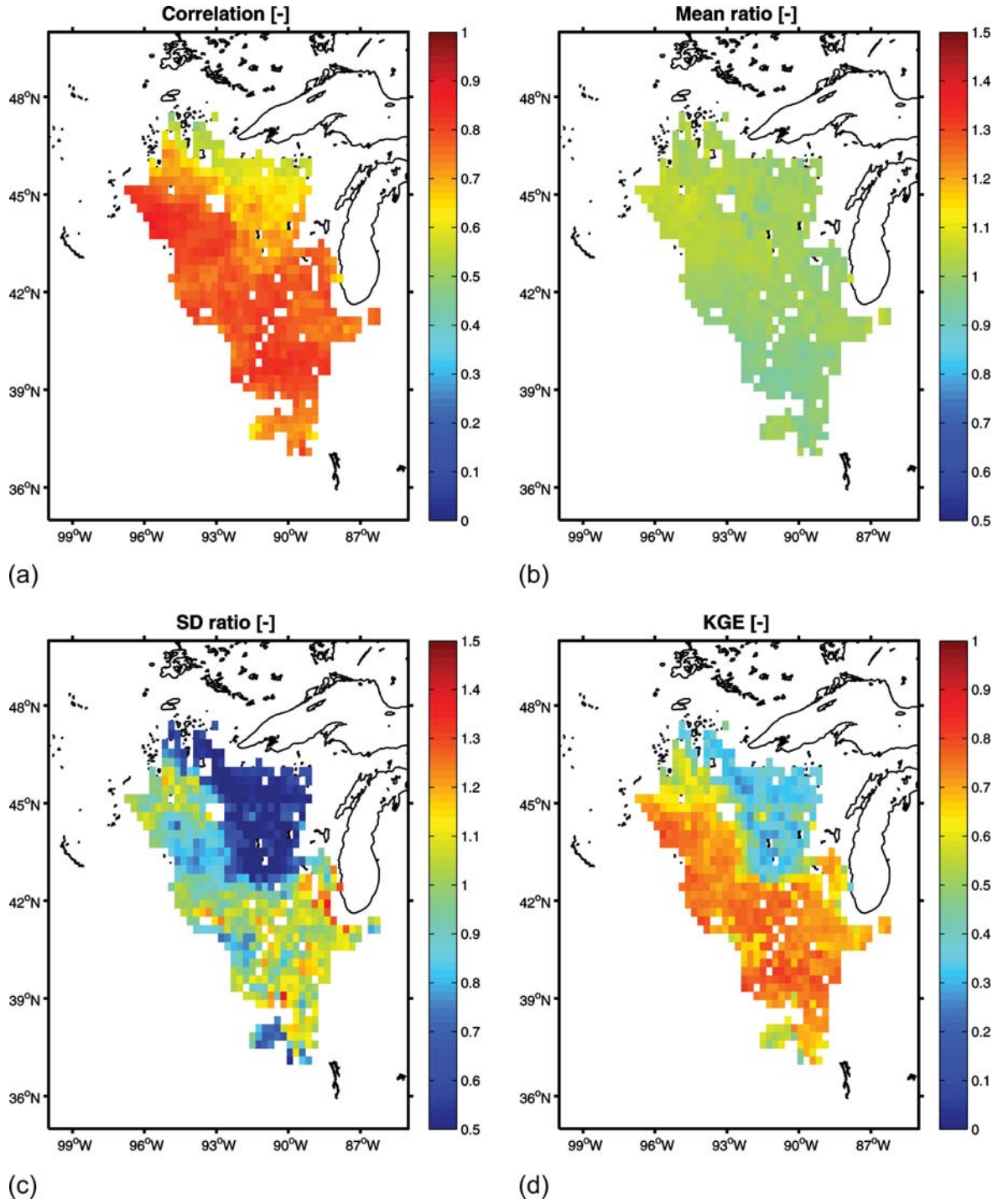


FIG. 10. The 2011 annual mean (a) correlation $[-]$, (b) mean ratio $[-]$, (c) standard deviation ratio $[-]$ and (d) KGE $[-]$ between SMOS TB and simulated TB (case 10) across all incidence angles, polarizations and orbits.

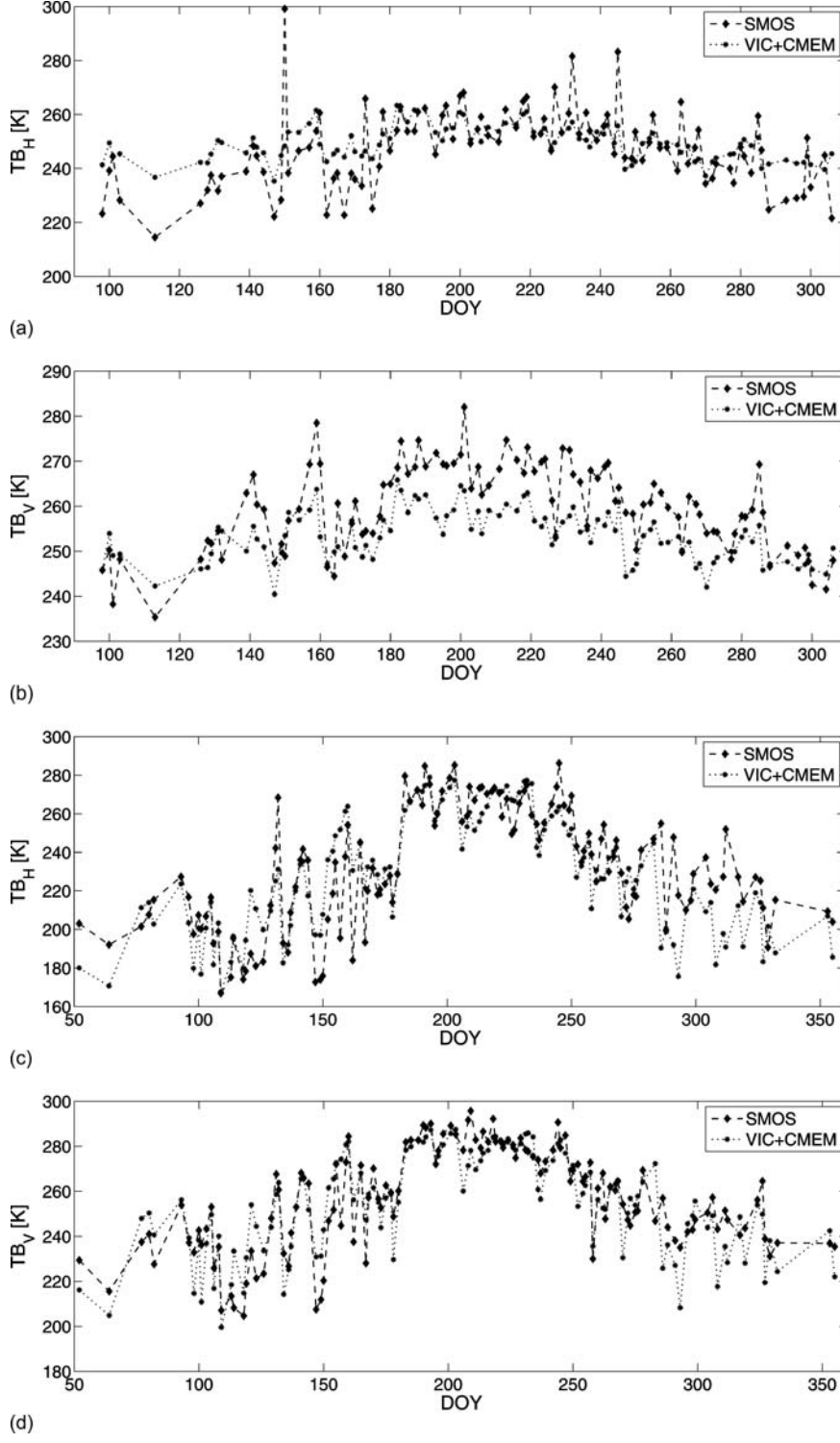


FIG. 11. 2011 time series of ascending TB [K] at 42.5° as observed by SMOS and simulated by VIC+CMEM (case 10), over (a, b) forest and (c, d) cropland grid cells, at (a, c) H-polarization and (b, d) V-polarization.